

2-DIMETHYLAMINOMETHYL-3-PYRIDINOL

Other names:	3-Pyridinol, 2-[(dimethylamino)methyl]- 2-[(dimethylamino)methyl]pyridin-3-ol
Inchi:	InChI=1S/C8H12N2O/c1-10(2)6-7-8(11)4-3-5-9-7/h3-5,11H,6H2,1-2H3
InchiKey:	NUMYETXZBQVFDX-UHFFFAOYSA-N
Formula:	C8H12N2O
SMILES:	CN(C)Cc1ncccc1O
Mol. weight [g/mol]:	152.20

Physical Properties

Property code	Value	Unit	Source
hf	-29.40	kJ/mol	Cheméo Relay (1.0)
ie	7.95	eV	Cheméo Relay (1.0)
logp	0.849		Crippen Method
mcvol	125.650	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	371.20	K	0.50	NIST Webbook

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C2168130&Units=SI>

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

hf:	Enthalpy of formation at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tbrp:	Boiling point at reduced pressure

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